Cyromazine 66215-27-8 | DTXSID6023999

Model Performance

Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 1.52e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.78e-01

Confidence level: 6.33e-01

Nearest Neighbors from the Training Set

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2-PTERIDINAMINE

Measured: 5.04e-03 Predicted: 1.72e-02

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Adenine

Measured: 7.62e-03 Predicted: 1.56e-02 Image not found

Melamine

Measured: 2.56e-02 Predicted: 7.17e-03